QUANTITATIVE CHEMICAL MASS TRANSFER IN COASTAL SEDIMENTS DURING EARLY DIAGENESIS: EFFECTS OF BIOLOGICAL TRANSPORT, MINERALOGY, AND FABRIC

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LONG-TERM GOAL

The long-term goal of the study is to develop a better mechanistic and quantitative understanding of the effects of biologically-enhanced transport, mineralogy, sediment fabric, and particle surface chemistry on the biogeochemical dynamics of coastal marine sediments.

OBJECTIVES

Objectives of the study are to (1) develop robust mathematical representations for sediment mixing, irrigation and sediment fabric, (2) parameterize transport and fabric functions using tracer experiments, high-resolution deterministic and stochastic submodels, measured profiles of physical and chemical properties of sediments plus pore waters, and high-resolution imaging of sediment fabric and statistical analysis of burrow networks, (3) incorporate the transport and fabric functions in an existing computer code for multicomponent reactive transport in aquatic sediments, and (4) perform sensitivity analyses and simulations.

APPROACH

Due to the complexity of the chemical, biological, and physical dynamics of coastal marine sediments, the development of quantitative models for mass transfer and sediment biogeochemistry requires an integrated field, laboratory, and computational approach. To this end an interdisciplinary consortium was formed which includes investigators from Naval Research Laboratory (Dawn Lavoie), University of Southern Mississippi (Yoko Furukawa), Scripps Institution of Oceanography (Barbara Ransom) and Georgia Institute of Technology (Philippe Van Cappellen). Georgia Tech is primarily responsible for the numerical modeling work.

The theoretical and computational efforts focus on the development of multi-dimensional stochastic models for biologically-enhanced solute and particle transport. The stochastic realizations are used to define average vertical transfer functions for irrigation and bioturbation, and constrain the horizontal spatial scales over which the one-dimensional functions are valid.

The vertical transfer functions are incorporated into the one-dimensional reactive transport model for early diagenesis, STEADYSED. This model fully accounts for the reaction couplings among the reactive species of C, O, N, S, Ca, Fe and Mn. It is used to simulate vertical distributions of chemical species and reaction rates in sediments, as well as to calculate benthic plus burial fluxes under variable depositional conditions at the seafloor.

WORK COMPLETED

STEADYSED was upgraded by representing the rates of $CaCO_3$ dissolution and precipitation in the continuity equations. The user can choose from a number of kinetic models for $CaCO_3$.

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A sensitivity analysis was performed with STEADYSED, under boundary conditions representative of coastal marine depositional environments, in order to quantify the importance of bio-irrigation on exchanges between sediments and the water column.

First steps were taken in the development of a two-dimensional (2-D) stochastic model for random vertical sediment burrowing by macrofauna. Based on numerous realizations of the stochastic burrow model, the average depth distribution of available burrow surface area (a proxy for the exchange coefficient), plus the deviation from the average are calculated. In this manner a statistical, rather than a deterministic, description of sediment burrowing is achieved.

RESULTS

Simulations show that by explicitly including $CaCO_3$ dissolution, the pore waters are buffered against large decreases in pH. The calculated pH distributions are consistent with those measured by micro-electrodes in the field. More simulations are needed to fully assess the effects of $CaCO_3$ precipitation. Results so far highlight the potential for using the vertical pH distribution as a diagnostic indicator of biogeochemical processes in sediments.

The sensitivity analysis indicates that benthic exchange fluxes of most solutes in nearshore marine systems are dominated by irrigation. Because of high rates of oxygen reduction in organic-rich coastal sediments, the contribution of molecular diffusion to benthic uptake of O_2 may in some cases be of the same order of magnitude or even larger than that of irrigation. The results emphasize the fundamental importance of pore water irrigation by macrofauna in controlling solute exchanges between sediments and the water column in coastal environments.

Burrowing strategies and environmental constraints that direct the activity of macrofauna can be represented by probability distributions for burrow length and burrow shape. Efforts in the near future will therefore focus on the formulation of appropriate "ecophysiological" distributions.

IMPACT/APPLICATIONS

A comprehensive reactive transport model for early diagenesis has many potential applications. By including more realistic representations of biological transport (bioturbation and irrigation) and mineral-organic interactions, it will be possible to examine the effects of these processes on the preservation of organic matter and the evolution of textural properties. A comprehensive model will also allow one to simulate the response of chemical mass transfer fluxes and reaction rates to a variety of natural and anthropogenic perturbations of the normal depositional regime, for example, input of pollutants, attempts at reclamation, eutrophication, storm events, changes in land use, and engineering projects.

TRANSITIONS

STEADYSED version 1.0 is available as public domain software on the P.I.'s server. Approximately 25 researchers have downloaded the program for use in a variety of applications.

RELATED PROJECTS

1. "Trace Metal Dynamics in Reducing Sediments: Determination of Adsorption and Coprecipitation on Undisturbed Sediment Core Sections Using a Plug Flow-Through Reactor" (P.I. Van Cappellen, EPA). The kinetic and thermodynamic parameters that are measured in this study are being incorporated into a trace metal subroutine which is coupled to STEADYSED.
2. "Biogeochemistry of Anaerobic Environments: An Integrated Geochemical and Microbiological Study of Dissimilatory Iron and Sulfate Reduction" (P.I.s Van Cappellen and DiChristina, NSF). This study

investigates the geochemical and microbial controls on two major anaerobic pathways of organic matter degradation in coastal marine sediments.

REFERENCES

An overview of projects on biogeochemistry can be found at www.gatech.edu/eas/bae.html.